

Nuclear Electron Capture in a Plasma

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Abstract

We consider the electron density at the position of an ion of charge Ze in a plasma under conditions approximating those in the core of the sun. Numerical calculations have shown that the plasma effects on the density, over and above the ordinary Coulomb factors that are obtained in the absence of electron-electron interactions, are well represented by a reduction factor, $\exp\{-Ze^2\beta\kappa_D\}$, where β is the inverse temperature and κ_D is the Debye wavelength. Although this factor is the direct analogue of the Salpeter enhancement factor for the fusion rates in stars, the elementary considerations that establish it in the fusion case are not applicable to the determination of the electron density and the resulting electron capture rates. We show analytically, through a sum rule that leads to a well-defined perturbative approach, that in the limit of Boltzmann statistics the Salpeter factor indeed provides the leading correction. We estimate residual effects, both from Fermi statistics and from short range terms.

I. INTRODUCTION AND SUMMARY

The purpose of this paper is to provide a clear and rigorous treatment of the process of nuclear electron capture in a plasma within the mean field approximation.

It is illuminating to begin by reviewing the effects of the surrounding plasma on the fusion of positively charged ions. The experience in looking at these plasma effects under solar (or weak screening) conditions is that the correction calculated by Salpeter (1954) is considerably larger than any other effect. The essence of this correction is replacement of the Coulomb potential by the Debye screened potential. Since the classical turning point for the ionic barrier penetration is at a much smaller radius than the Debye radius, it suffices to evaluate a screening energy correction to the barrier penetration problem, an energy determined by taking the difference between the unscreened and screened potentials as r approaches zero. This energy difference is given by $\Delta E = -e^2 Z_1 Z_2 \kappa_D$ where Z_1 and Z_2 are the charges of the two nuclei. Then the obvious statistical argument gives the enhancement factor $\exp\{\beta e^2 Z_1 Z_2 \kappa_D\}$.

However it is not at all clear that this factor applies, as a matter of principle, to the plasma corrections to the electron density at a nucleus. One difference is that we now deal with an attraction rather than a repulsion, so that at least the language of the above qualitative description must be changed. But the important difference is that the thermal wavelength for the electron is much greater than that for the ion; for the solar problem it is only a little smaller than the Debye length. The WKB approximation gives a theoretical justification for considering the outer regions of the electronic cloud surrounding the nucleus to be governed by a classical statistical distribution determined by the temperature, chemical potential, and local electrostatic potential. But for an electron at a distance from the nucleus of one wavelength, the WKB approach is not applicable. Thus the simplest argument for the Salpeter factor (now a suppression) seems not to apply to the electron case.

Nevertheless, in the case of greatest current interest in solar processes, electron capture in ${}^7\text{Be}$, more detailed calculations of electronic wave functions have given screening related

reductions to the $r = 0$ electron density that are only slightly less than would have resulted from a Salpeter formula. In these calculations, beginning with those of Iben, Kalata and Schwarz (1967), then sharpened by Bahcall and Moeller (1969), and by Johnson, Kolbe, Koonin, and Langanke (1992), the screening induced reduction comes about in an way that we describe below.

1) The Saha equation is used to determine the degree of occupation of the bound states in ${}^7\text{Be}$ in the medium assuming pure Coulomb electron-ion forces; for example, there turns out to be roughly a 20% probability of occupation for both the $m = \pm 1/2$ 1S states (Iben, Kalata, and Schwartz 1967). Leaving out screening, the 1S states give a contribution of about 35% of the continuum contribution to the $r = 0$ electron density at the nucleus. The higher bound states in this picture have appreciable occupation as well, and contribute another 6% of the continuum value.

2) When Debye screening is introduced, as shown by Bahcall and Moeller (1967), the contribution of the continuum states to the $r = 0$ density is changed by a very small amount, of the order of 1%.

3) The screening reduces the occupation factor for the 1S state by a bit; it changes the wave function at $r = 0$ of this state by quite a bit more, with the end result that in the screened problem the 1S contribution is reduced to about 20% of the continuum contribution. As pointed out by Gruzinov and Bahcall (1997), combining this reduction with the complete removal of the higher bound states gives a net reduction due to screening that is quite close to that predicted by a Salpeter formula.

Gruzinov and Bahcall address the problem through a quantum diffusion equation elucidated by Feynman (1990) and applicable in the case of Boltzmann statistics. The approach provides both a qualitative understanding of why the Salpeter factor is a good approximation in the high temperature limit and a computational framework for incorporating the effects of classical plasma fluctuations. Unlike the other approaches described above, it does not need to calculate occupation probabilities from the Saha equation. (The Saha equation, and indeed the “percentage occupancy” that it describes, are not well defined once electrons

interact with themselves.)

In the present work, which we view as complementary to that of Gruzinov and Bahcall, we show analytically that in the Boltzmann limit the Salpeter correction is indeed the leading correction in a well defined perturbative approach. Furthermore, in the leading order of approximation, Fermi statistics can be maintained at little cost, since the generalization of the Salpeter multiplicative factor, in going from pure Coulomb to screened, is a simple displacement of the electron chemical potential μ_e . Thus the Salpeter factor is regained in the Maxwell-Boltzmann limit in which everything is proportional to $\exp\{\beta\mu_e\}$.

In establishing these results we do not need to separate bound from continuum parts, or use a Saha equation. We have also calculated leading small corrections to this basic result. In contrast to the fluctuation corrections of Gruzinov and Bahcall (1997), the additional terms depend on the quantum mechanics of the plasma.

We turn now to describe our results; the mathematical details that support them are relegated to the Appendix.

As in the previous work, we exploit the large nucleus – electron mass ratio so that the nucleus may be treated as a fixed point of charge Ze , with the capture rate proportional to the electron density at this point which we take to be the coordinate origin. In many-body field theory language, this density is given by the thermal ensemble average

$$D(\beta, \mu_e) = \langle \psi^\dagger(0)\psi(0) \rangle_\beta. \quad (1.1)$$

Here¹ $\beta = 1/T$ is the inverse temperature and μ_e is the chemical potential of the electrons. This general formula includes all possible corrections resulting from the electron-plasma interactions to the electron density at the nucleus. The thermal expectation value of the field operators is the coincident point limit of the two-point, single-particle electron Green's function, including all plasma interactions as well as having an additional fixed point charge Ze

¹We employ energy units for the temperature T and use natural units in which Planck's constant $\hbar = 1$.

at the coordinate origin. This single-particle Green's function has a standard representation in terms of the single-particle irreducible electron self-energy function Σ . The self-energy function may be divided into two parts: 1. A part that contains all the terms depicted by all the graphs which end with a single Coulomb photon line connected to the electron line. These graphs define an effective, external, local screened potential $V_S(r)$ in which the electron propagates. In the small Z , dilute plasma limit, this potential is the Coulomb potential produced by the heavy nucleus as modified by the plasma polarization accounted for by the familiar ring graph sum. In general, however, $V_S(r)$ contain all possible interactions of the heavy nucleus with the plasma and all possible plasma interactions, except that all these interactions are communicated in the end to the electron by a single Coulomb photon exchange. 2. A part that contains all other plasma effects. These entail at least two Coulomb photon lines attached to the electron line. The leading correction in this part is the exchange energy correction that is familiar in the Hartree-Fock description of atoms.

In this paper, we shall investigate only the corrections to the electron density at the nucleus resulting from the screened potential² $V_S(r)$. Thus the dynamics of the electron field operator $\psi(\mathbf{r}, \tau)$ is governed by the screened potential $V_S(r)$ with no other particle-particle interactions. The electron field operator satisfies the simple Schrödinger equation for a particle in the potential $V_S(r)$. The Green's functions of the theory are of the same form as those in the completely non-interacting theory except that in their spectral representation, free-particle wave functions are replaced by the corresponding Schrödinger eigenfunctions in the potential $V_S(r)$. Hence, with no further approximation, the density reads

²Although we have given a precise definition of $V_S(r)$ in terms of the single-photon line reducible contribution to the electron self-energy function Σ , the following considerations apply to any local mean-field potential $V_M(r)$. However, any terms that are added to our definition of $V_S(r)$ must then be subtracted from the remainder of Σ , and the net effect of the resulting Σ must be shown to be small.

$$D_S(\beta, \mu_e) = \int dE n(E, \mu_e) |\psi_S(E; 0)|^2, \quad (1.2)$$

where the integration implies in addition a summation over possible discrete bound states, and where

$$n(E, \mu_e) = \frac{2}{e^{\beta(E - \mu_e)} + 1}, \quad (1.3)$$

with the 2 in the numerator accounting for the 2 spin states; $\psi_S(E; 0)$ is the properly normalized Schrödinger wave function for energy E . It should be emphasized that the result (1.2) automatically accounts for the proper weighting of the bound state contributions, no additional “Saha-like” reasoning need be done.

In the limit in which the screened potential is replaced by the Coulomb potential

$$V_C(r) = -\frac{Ze^2}{r}, \quad (1.4)$$

we have the continuum wave functions for $0 \leq E < \infty$ with

$$|\psi_C(E; 0)|^2 = \frac{Zm}{\pi a_0} \frac{1}{1 - e^{-2\pi\eta}}, \quad (1.5)$$

in which m is the electron mass, $E = p^2/2m$, $a_0 = 1/e^2m$ is the electron Bohr radius, and $\eta = Z/a_0p$ is the usual Coulomb parameter. In addition, there is the infinite set of bound state wave functions giving

$$|\psi_n(0)|^2 = \frac{Z^3}{\pi a_0^3 n^3}, \quad (1.6)$$

with the bound state energies

$$E_n = -\frac{Z^2 e^2}{2a_0 n^2}. \quad (1.7)$$

We shall denote the the electron density at the nucleus in this Coulomb limit by $D_C(\beta, \mu_e)$, with

$$D_C(\beta, \mu_e) = \sum_{n=1}^{\infty} |\psi_n(0)|^2 n(E_n, \mu_e) + \int_0^{\infty} dE n(E, \mu_e) |\psi_C(E; 0)|^2. \quad (1.8)$$

We shall express the corrections in terms of the electron density $\langle n_e \rangle_\beta$ in the plasma far away from the capturing nucleus. Neglecting interacting plasma effects, this density is given by

$$\begin{aligned} \langle n_e \rangle_\beta &= \int \frac{(d^3 \mathbf{p})}{(2\pi)^3} n(E, \mu_e) \\ &= 2\lambda_e^{-3} e^{\beta\mu_e} \left[1 - \frac{1}{2\sqrt{2}} e^{\beta\mu_e} + \frac{1}{3\sqrt{3}} e^{2\beta\mu_e} + \dots \right], \end{aligned} \quad (1.9)$$

where, in the second line λ_e is the electron thermal wavelength defined by

$$\lambda_e = \sqrt{\frac{2\pi\beta}{m}}, \quad (1.10)$$

and we have expanded the denominator in the Fermi-Dirac distribution $n(E, \mu_e)$, performed the momentum integrals, and kept the first two corrections to the classical statistics limit. For our numerical corrections, we shall use the parameters stated by Gruzinov and Bahcall (1997) which describe the solar interior at a distance 6% away from the sun's center. We shall also write the parameters in essentially atomic units, except that we shall display the units. Thus we take

$$\beta = 0.0215 \left(a_0/e^2 \right), \quad (1.11)$$

corresponding to a temperature $T = (e^2/a_0)/0.0215 = 1.27$ KeV. This temperature gives

$$\lambda_e = 0.368 a_0. \quad (1.12)$$

The electron density is taken to be

$$\langle n_e \rangle_\beta = 9.10/a_0^3, \quad (1.13)$$

which gives by Eq. (1.9)

$$e^{\beta\mu_e} = 0.245. \quad (1.14)$$

The resulting Debye wave number defined³ by $\kappa_D^2 = 4\pi e^2 \beta 2\langle n_e \rangle_\beta$ reads

$$\kappa_D = 2.22 / a_0, \quad \kappa_D^{-1} = 0.451 a_0. \quad (1.15)$$

We shall first demonstrate that the electron density $D_D(\beta, \mu_e)$ at the nucleus for the Debye potential

$$V_D(r) = -\frac{Ze^2}{r} e^{-\kappa_D r} \quad (1.16)$$

may be expressed, to a good approximation, in terms of the Coulomb limit and then describe the correction that arise from a more accurate treatment of the screened potential. This relationship between the Debye and Coulomb density follows from a sum rule (A25) proved in the Appendix⁴,

$$\int dE \left\{ |\psi_D(E; 0)|^2 - |\psi_C(E'; 0)|^2 \right\} = \frac{Z\kappa_D^2}{16\pi a_0}, \quad (1.17)$$

where

$$E' = E - Ze^2 \kappa_D. \quad (1.18)$$

We make use of this sum rule to write

$$D_D(\beta, \mu_e) = \int dE n(E, \mu_e) |\psi_C(E'; 0)|^2 + R_D(\beta, \mu_e), \quad (1.19)$$

in which

$$R_D(\beta, \mu_e) = \int dE [n(E, \mu_e) - n(0, \mu_e)] \left\{ |\psi_D(E; 0)|^2 - |\psi_C(E'; 0)|^2 \right\} + \frac{Z\kappa_D^2}{16\pi a_0} n(0, \mu_e) \quad (1.20)$$

³Accounting for Fermi-Dirac statistics, the electron contribution to the Debye wave number is given by $\kappa_{D,e}^2 = 4\pi e^2 \partial \langle n_e \rangle_\beta / \partial \mu_e$. This correct definition reduces the total Debye wave number by 2%, but it entails only a negligible 1/2% effect for ${}^7\text{Be}$ capture.

⁴Note that the convergence of the integration for $E \rightarrow \infty$ is delicate: The two squared wave functions must be subtracted at the same energy; their separate integrals do not exist.

will be shown to be a quite small correction. Translating the energy in the integration in Eq. (1.19) to remove the displacement shown in the definition (1.18) of E' and noting that this translation just shifts the value of the chemical potential μ_e in the weight (1.3), we see that Eq. (1.19) may be expressed as

$$D_D(\beta, \mu_e) = D_C(\beta, \mu_e - Ze^2\kappa_D) + R_D(\beta, \mu_e). \quad (1.21)$$

To keep simple analytic forms, we shall express the corrections in terms of the bulk electron density $\langle n_e \rangle_\beta$ in the plasma. Including the first non-classical correction,

$$\frac{Z\kappa_D^2}{16\pi a_0} n(0, \mu_e) = \langle n_e \rangle_\beta \frac{Z\kappa_D^2 \lambda_e^3}{16\pi a_0} \left[1 - \left(1 - \frac{1}{2\sqrt{2}} \right) e^{\beta\mu_e} \right]. \quad (1.22)$$

Since the sum rule implies that on the average the difference between $|\psi_S(E; 0)|^2$ and $|\psi_C(E'; 0)|^2$ is small, the integral in $R_D(\beta, \mu_e)$,

$$I_D(\beta\mu_e) = \int dE \left\{ |\psi_D(E; 0)|^2 - |\psi_C(E'; 0)|^2 \right\} [n(E, \mu_e) - n(0, \mu_e)], \quad (1.23)$$

should give a small contribution. Moreover, the sum rule has been used to subtract $n(0, \mu_e)$ from $n(E, \mu_e)$, and this difference becomes large only at energies that are large on the atomic scale, large energies that are on the order of the temperature T . At large energies, the terms in the perturbative development of the wave functions converges rapidly and so this high-energy contribution can be computed analytically. Said another way, this contribution gives the leading term for small β and, in view of Eq. (1.11), β is indeed small in the relevant atomic units. For moderate energies, the integration in Eq. (1.23) gives terms that are linear in β . The high-energy contribution obtained in Eq.(A31) of the Appendix is of order $\sqrt{\beta}$ which is larger for small β . Since the Fermi-Dirac corrections to the Maxwell-Boltzmann limit are small, we include only the first correction in this high-energy contribution. Combining the result of Eq. (A31) with Eq. (1.22), we obtain the leading correction to the remainder

$$R_D(\beta, \mu_e) = \langle n_e \rangle_\beta \frac{Z\kappa_D \lambda_e^3}{2\pi a_0^2} \left\{ \frac{a_0 \kappa_D}{8} \left[1 - \left(1 - \frac{1}{2\sqrt{2}} \right) e^{\beta\mu_e} \right] + \left(\frac{3Z}{4} - \frac{a_0 \kappa_D}{12} \right) \sqrt{\frac{1}{\pi} \frac{\beta \kappa_D^2}{2m}} \left[1 - \frac{3\sqrt{2}}{4} e^{\beta\mu_e} \right] \right\}. \quad (1.24)$$

For the parameters listed above,

$$R_D(\beta, \mu_e) = 0.018 Z \{0.28 [1 - 0.16] + 0.098 (Z - 0.25)[1 - 0.26]\} \langle n_e \rangle_\beta. \quad (1.25)$$

For $Z = 4$, this gives $R_D(\beta, \mu_e) = 0.04 \langle n_e \rangle_\beta$, while as we shall see shortly, the corresponding capture density $R(\beta \mu_e)$ is about $4 \langle n_e \rangle_\beta$. Thus this leading additional correction to the basic correction provided by the Salpeter factor is only 1%, and any further corrections should be smaller yet.

The Debye potential (1.16) that we have been using has the linear term $-Ze^2 \kappa_D r$ in its short distance limit. As the work in the Appendix shows, it is this term that gives the non-vanishing value to the right-hand side of the sum rule (1.17). No linear term in r appears in the correct screened potential $V_S(r)$ since such a term would give rise to an unphysical screening charge density $[-\nabla^2 r = -1/r]$. However, the corrections that remove this linear term at extremely short distances arise from wave numbers in the Fourier transform of the potential, $\tilde{V}_S(k)$, that are of order $1/\lambda_s$, where λ_s is the thermal wave number of a species s particle in the plasma. For the ions in the plasma, the distance λ_s is very small in comparison with the other relevant distances in our problem, and this cut off is not important. Indeed, the work of the Appendix shows that this effect for the ions in the plasma is of order m/M_s relative to the small corrections that we have already displayed. But for the electrons in the plasma, the cut off at λ_e is as important as the other corrections that we have displayed. This effect of the electrons in the plasma is computed in the Appendix in the dilute plasma limit and to leading order in the small parameter $\beta Z^2 e^2 / 2a_0$. In these limits, the correction given by Eq. (A41) reads

$$\Delta D(\beta, \mu_e) = \langle n_e \rangle \frac{Z \kappa_D^2 \lambda_e^3}{8\pi^3 a_0} I, \quad (1.26)$$

where I is a parameter integral that has the numerical value $I = 1.105$. For the parameter values used before, this gives a negligible effect:

$$\Delta D(\beta, \mu_e) = 0.001 Z \langle n_e \rangle_\beta. \quad (1.27)$$

We have now shown that to within an accuracy on the order of 1%, the screened electron density $D_S(\beta, \mu_e)$ is given by the simple Coulomb density, but with a translated chemical potential, $D_C(\beta, \mu_e - Ze^2\kappa_D)$. It remains to evaluate this main term using Eq. (1.8). Following Gruzinov and Bahcall, we define an enhancement factor which is the ratio of the electron density at the nucleus calculated in various schemes to the average electron density given in Eq. (1.9),

$$w = \frac{D(\beta, \mu_e)}{\langle n_e \rangle_\beta}. \quad (1.28)$$

We denote by w_S the complete result of the shifted chemical potential Coulomb density including the effect of Fermi-Dirac statistics and including the small correction shown in Eq. (1.25). The same quantity, but using Maxwell-Boltzmann statistics, is labeled $w_{S,B}$. The ratio with no screening corrections, the simple Coulomb result is written as w_C for the case of the full Fermi-Dirac statistics and $w_{C,B}$ in the Maxwell-Boltzmann limit. Finally, the results of Gruzinov and Bahcall (1997) will be denoted as w_{GB} . As discussed previously, we use the parameters given by Gruzinov and Bahcall in order to compare our results with theirs. The ratios given by the various schemes as well as a direct comparison with their results are displayed in the following table:

Z	1	2	3	4	5	6
w_S	1.38	1.89	2.63	3.67	5.12	7.19
$w_{S,B}$	1.39	1.94	2.72	3.84	5.46	7.82
w_C	1.43	2.05	2.96	4.29	6.22	9.04
$w_{C,B}$	1.45	2.11	3.10	4.59	6.84	10.3
w_{GB}	1.39	1.94	2.73	3.85	5.50	7.90
$\frac{w_{S,B}}{w_{GB}}$	1.00	1.00	1.00	1.00	0.99	0.99
$\frac{w_S}{w_{S,B}}$	0.99	0.97	0.97	0.96	0.94	0.92

The ratio of ratios $w_{S,B}/w_{C,B}$ is essentially the Salpeter factor $\exp\{-\beta Ze^2\kappa_D\}$ which varies from 0.95 for $Z = 1$ through 0.83 for $Z = 4$ to 0.75 for $Z = 6$. The small term

$R_D(\beta, \mu_e)$ displayed in Eq. (1.25) gives a correction to $w_{S,B}$ that varies from 0.4 % for $Z = 1$ through 1 % for both $Z = 4$ and $Z = 6$. The next-to-last row in the table, the ratio of ratios $w_{S,B}/w_{GB}$ should be precisely unity if our approximations were without error and the computation of Gruzinov and Bahcall were precise.⁵ The last row in the table, the ratio of ratios $w_S/w_{S,B}$, displays the effect of Fermi statistics on the capture rate.

We conclude that the numbers from the calculations cited earlier are sufficiently accurate to determine the electron capture in rate in ${}^7\text{Be}$ to the precision needed for analysis of future solar neutrino results. The development presented in the present work first provides a rigorous basic formulation that unambiguously describes the electron density at the nucleus in the screened field approximation with no need of any considerations of the Saha type. It then gives an analytical way of understanding the main features of previous calculations, as well as an approach that may be useful in addressing related problems in the future.

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⁵We have recalculated Gruzinov and Bahcall’s mean field values and found small discrepancies for $Z = 1$ and $Z = 6$. The corrected results are given in our table.

APPENDIX A: SUM RULE, HIGH-ENERGY BEHAVIOR

Here we shall derive the sum rule and other results used in the text. This will be done by examining the high-energy behavior of S-wave, radial Green's functions defined by the inhomogeneous differential equation

$$\left[-\frac{1}{2m} \frac{d^2}{dr^2} + V(r) - E \right] \mathcal{G}(E; r, r') = \delta(r - r') \quad (\text{A1})$$

together with outgoing wave boundary conditions. In particular, we shall first compare the Green's function $\mathcal{G}_D(E; r, r')$ for the Debye potential

$$V_D(r) = -\frac{Ze^2}{r} e^{-\kappa_D r}, \quad (\text{A2})$$

with the Green's function $\mathcal{G}_C(E'; r, r')$ at the translated energy

$$E' = \frac{p'^2}{2m} = E - Ze^2 \kappa_D, \quad (\text{A3})$$

for the Coulomb potential

$$V_C(r) = -\frac{Ze^2}{r}. \quad (\text{A4})$$

This comparison is most easily done by noting that

$$\mathcal{G}_D(E; r, r') = \mathcal{G}_C(E'; r, r') - \int_0^\infty d\bar{r} \mathcal{G}_C(E'; r, \bar{r}) \Delta V(\bar{r}) \mathcal{G}_D(E; \bar{r}, r'), \quad (\text{A5})$$

where

$$\begin{aligned} \Delta V(r) &= V_D(r) - V_C(r) + E' - E \\ &= -Ze^2 \left[\frac{1}{r} (e^{-\kappa_D r} - 1) + \kappa_D \right]. \end{aligned} \quad (\text{A6})$$

This integral equation defines a Green's function $\mathcal{G}_D(E; r, r')$ which obeys the proper differential equation (A1) with the Debye potential $V_D(r)$, and this Green's function is defined with outgoing wave boundary conditions if these boundary conditions are obeyed by the Coulomb Green's function $\mathcal{G}_C(E'; r, r')$.

The high-energy behavior of the Green's function may be obtained by iterating the integral equation (A5) to form the perturbative series

$$\mathcal{G}_D(E; r, r') = \mathcal{G}_C(E'; r, r') - \int_0^\infty d\bar{r} \mathcal{G}_C(E'; r, \bar{r}) \Delta V(\bar{r}) \mathcal{G}_C(E'; \bar{r}, r') + \dots \quad (\text{A7})$$

The high-energy limit probes the short-distance limit of the perturbation, $\Delta V(\bar{r}) \rightarrow -Ze^2\kappa_D^2 \bar{r}/2$, and the high-energy limit of the Coulomb Green's function which (by simple dimensional reasons) has an overall factor of m/p . The Fourier transform involved in the \bar{r} -integration of the leading \bar{r} term in $\Delta V(\bar{r})$ gives rise, in the high-energy limit to another factor of $1/p^2$. Thus the successive terms in the perturbative development are smaller by a factor of $1/p^3$ in the high-energy limit, and, as we shall see, it suffices for our purposes to retain only the first correction as shown in Eq. (A7).

The Coulomb Green's function may be constructed in terms of solutions to the S-wave Coulomb radial Schrödinger equation, the homogeneous counterpart of the Green's function differential equation (A1). These solutions are confluent hypergeometric functions which have standard integral representations. The functions we need may be defined by

$$A(E; r) = -2ipr \int_0^\infty dt e^{ipr(2t+1)} t^{-i\eta} (1+t)^{i\eta}, \quad (\text{A8})$$

and

$$B(E; r) = \frac{r}{\Gamma(1-i\eta)\Gamma(1+i\eta)} \int_0^1 du e^{-ipr(2u-1)} u^{-i\eta} (1-u)^{i\eta}, \quad (\text{A9})$$

where

$$\eta = \frac{Ze^2m}{p} = \frac{Z}{pa_0}. \quad (\text{A10})$$

It is a straight forward matter to check that these integral representations obey the Coulomb S-wave radial Schrödinger equation⁶. It is also not difficult to establish the limits

$$r \rightarrow 0 : \quad A(E; r) \rightarrow 1, \quad (\text{A11})$$

⁶The application of this differential equations results in integrals of total derivatives that vanish.

$$r \rightarrow 0 : \quad B(E; r) \rightarrow r , \quad (\text{A12})$$

and the asymptotic behavior

$$r \rightarrow \infty : \quad A(E; r) \rightarrow e^{ipr} \left(\frac{i}{2pr} \right)^{-i\eta} \Gamma(1 - i\eta) . \quad (\text{A13})$$

Thus $B(E; r)$ is the regular solution and $A(E; r)$ has outgoing waves. Moreover, the $r \rightarrow 0$ limit and the constancy of the Wronskian give

$$W = \frac{dA(E; r)}{dr} B(E; r) - A(E; r) \frac{dB(E; r)}{dr} = -1 . \quad (\text{A14})$$

Accordingly, the Coulomb Green's function has the construction

$$\mathcal{G}_C(E; r, r') = 2m A(E; r_{>}) B(E; r_{<}) , \quad (\text{A15})$$

where $r_{>}, r_{<}$ are the greater and lessor of r, r' .

The results that we need are obtained by examining the high-energy behavior of

$$\Delta(E) = \lim_{r, r' \rightarrow 0} \frac{1}{r} [\mathcal{G}_D(E; r, r') - \mathcal{G}_C(E'; r, r')] \frac{1}{r'} . \quad (\text{A16})$$

To the order of accuracy that we need, Eq. (A7) and the Coulomb Green's function construction (A15) give

$$\Delta(E) = -(2m)^2 \int_0^\infty dr \Delta V(r) A(E; r)^2 . \quad (\text{A17})$$

In the high-energy limit, the Coulomb parameter $\eta = Z/pa_0$ becomes small, and so the integral representation (A8) gives

$$A(E'; r)^2 \approx e^{2ip'r} - 4p'r \eta' \int_0^\infty dt e^{2ip'r(1+t)} \ln \left(\frac{t}{1+t} \right) . \quad (\text{A18})$$

Moreover, since the high-energy limit involves only the short-distance behavior of the perturbing potential, we may approximate

$$\Delta V(r) \approx -Ze^2 \left[\frac{1}{2} \kappa_D^2 r - \frac{1}{6} \kappa_D^3 r^2 \right] . \quad (\text{A19})$$

To our order, only the first term here contributes in the η' correction to $A(E'; r)^2$, and we have

$$\Delta(E) = Ze^2(2m)^2 \left\{ \frac{\kappa_D^2}{2(2ip')^2} + \frac{\kappa_D^3}{3(2ip')^3} + \frac{4\kappa_D^2 p' \eta'}{(2ip')^3} \int_0^\infty \frac{dt}{(1+t)^3} \ln \left(\frac{t}{1+t} \right) \right\}. \quad (\text{A20})$$

The integral that appears here is reduced to an elementary integral by the variable change $1+t=1/x$. Thus, after a little algebra, we find that the leading high-energy limit is given by

$$E \rightarrow \infty : \quad \Delta(E) = -\frac{Z\kappa_D^2}{4a_0 E} + i\frac{Z}{a_0^3 E^{3/2}} A, \quad (\text{A21})$$

in which

$$A = \left[\frac{a_0^2 \kappa_D^2}{12} - \frac{3Za_0 \kappa_D}{4} \right] \sqrt{\frac{\kappa_D^2}{2m}} \quad (\text{A22})$$

To obtain the desired sum rule, we note that the Green's functions have a spectral representation. Since the radial functions that we have used are related to the total wave function by

$$\psi(E; r) = \frac{u(E; r)}{r} Y_0^0 = \frac{u(E; r)}{r} \frac{1}{\sqrt{4\pi}}, \quad (\text{A23})$$

this spectral representation yields

$$\frac{\Delta(E)}{4\pi} = \int d\bar{E} \frac{|\psi_S(\bar{E}; 0)|^2 - |\psi_C(\bar{E}; 0)|^2}{\bar{E} - E - i\epsilon}, \quad (\text{A24})$$

where the integration implicitly includes a sum over all bound states. In view of the high-energy limit (A21), we conclude that

$$\int dE \left\{ |\psi_S(E; 0)|^2 - |\psi_C(E; 0)|^2 \right\} = +\frac{Z\kappa_D^2}{16\pi a_0}, \quad (\text{A25})$$

which is the sum rule used in the text. Since

$$\text{Im} \frac{1}{\bar{E} - E - i\epsilon} = \pi \delta(\bar{E} - E), \quad (\text{A26})$$

we also have

$$|\psi_S(E; 0)|^2 - |\psi_C(E; 0)|^2 = \frac{\text{Im} \Delta(E)}{4\pi^2}, \quad (\text{A27})$$

which we shall now use to obtain the corrections presented in the text.

The result (A27) expresses the integral in the remainder $R_D(\beta, \mu_e)$ defined in Eq. (1.23) as

$$I_D(\beta, \mu_e) = \int dE \frac{\text{Im}\Delta(E)}{4\pi^2} [n(E, \mu_e) - n(0, \mu_e)] . \quad (\text{A28})$$

Since, in the relevant atomic units, the inverse temperature β is quite small, we shall evaluate this integral in the small β limit, which should give the leading correction. The integration over finite energies gives a result that is first order in β , but, as we shall soon see, the integration region of large β gives a larger contribution for small β , a contribution of order $\sqrt{\beta}$. This larger contribution is given by the high-energy limit (A21). Since the departure from classical statistics is small, we shall retain only the first-order correction in $\exp\{\beta\mu_e\}$ and thus compute

$$\begin{aligned} I_D(\beta\mu_e) &\approx \frac{ZA}{4\pi^2 a_0^3} 2e^{\beta\mu_e} \int_0^\infty \frac{dE}{E^{3/2}} [(e^{-\beta E} - 1) - e^{\beta\mu_e} (e^{-2\beta E} - 1)] \\ &= -\frac{ZA}{4\pi^2 a_0^3} 2e^{\beta\mu_e} 2\sqrt{\beta\pi} [1 - \sqrt{2}e^{\beta\mu_e}] . \end{aligned} \quad (\text{A29})$$

Using Eq. (1.9) to express this in terms of the bulk electron density gives

$$I_D(\beta\mu_e) \approx -\langle n_e \rangle_\beta \frac{Z\lambda_e^3}{2\pi a_0^3} \sqrt{\frac{\beta}{\pi}} \left[1 - \frac{3\sqrt{2}}{4} e^{\beta\mu_e} \right] , \quad (\text{A30})$$

with the result (A22) finally yielding

$$I_D(\beta\mu_e) \approx \langle n_e \rangle_\beta \frac{Z\kappa_D \lambda_e^3}{2\pi a_0^2} \left[1 - \frac{3\sqrt{2}}{4} e^{\beta\mu_e} \right] \left(\frac{3Z}{4} - \frac{a_0 \kappa_D}{12} \right) \sqrt{\frac{1}{\pi} \frac{\beta \kappa_D^2}{2m}} . \quad (\text{A31})$$

We turn at last to examine the correction to the electron density at the nucleus that comes from the difference between the Debye potential $V_D(r)$ and a more accurate screened potential $V_S(r)$. Since the two potentials have the same long-distance behavior, their difference becomes important only at high energies where the effects of the Coulomb interaction become small. Hence, a good estimate is obtained by replacing the Coulomb function $A(E'; r)$ by the plane wave $\exp\{ipr\}$ in Eq. (A17):

$$\bar{\Delta}_1(E) = -(2m)^2 \int_0^\infty dr e^{2ipr} \{V_S(r) - V_D(r)\} . \quad (\text{A32})$$

The Fourier transform of the screened potential may be written in the general form

$$\tilde{V}_S(k) = -Ze^2 \frac{4\pi}{k^2 + 4\pi\Pi(k)}. \quad (\text{A33})$$

With $4\pi\Pi(k) = \kappa_D^2$, this gives the Debye potential. Hence

$$\begin{aligned} V_S(r) - V_D(r) &= Ze^2 \int \frac{(d\mathbf{k})}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \frac{4\pi}{k^2 + \kappa_D^2} \frac{4\pi [\Pi(k) - \Pi(0)]}{k^2 + 4\pi\Pi(k)} \\ &\approx 8Ze^2 \int_0^\infty \frac{dk}{k^2} \frac{\sin kr}{kr} [\Pi(k) - \Pi(0)], \end{aligned} \quad (\text{A34})$$

where in the second approximate equality we have performed the angular integration and neglected the denominator corrections that are of order κ_D^2 and do not contribute to the leading high-energy behavior. Using

$$\int_0^\infty \frac{dr}{r} e^{2ipr} \sin kr = -\frac{i}{2} \ln \left[\frac{2p - k}{2p + k} \right], \quad (\text{A35})$$

and thus obtain

$$\text{Im } \bar{\Delta}_1(E) = \frac{16mZ}{a_0} \int_0^\infty \frac{dk}{k^3} [\Pi(k) - \Pi(0)] \ln \left| \frac{2p - k}{2p + k} \right|. \quad (\text{A36})$$

Again for simplicity using Maxwell-Boltzmann statistics, this gives the correction to the electron density at the nucleus of

$$\Delta D(\beta, \mu_e) = 2e^{\beta\mu_e} \int_0^\infty \frac{pdp}{m} \exp \left\{ -\beta \frac{p^2}{2m} \right\} \frac{\text{Im } \bar{\Delta}_1(E)}{4\pi^2}. \quad (\text{A37})$$

We now represent the plasma polarization function $\Pi(k)$ by its one-loop, ring graph approximation. Using the results of Brown and Sawyer, their Eq's. (A41) and (A42), we find that

$$\Pi(k) - \Pi(0) = \sum_s e_s^2 \beta \langle n_s \rangle_\beta \int_0^1 dt \left[\exp \left\{ -\frac{\beta k^2}{2M_s} t(1-t) \right\} - 1 \right], \quad (\text{A38})$$

where the sum runs over all species s of the particles in the plasma. We perform the integration over p by writing $k = 2px$ to obtain

$$\begin{aligned} \Delta D(\beta, \mu_e) &= -2e^{\beta\mu_e} \sum_s e_s^2 \beta \langle n_s \rangle_\beta \frac{Z}{2\pi^2 a_0} \int_0^\infty \frac{dx}{x^3} \int_0^1 dt \\ &\quad \ln \left| \frac{1-x}{1+x} \right| \ln \left[1 + 4x^2 t(1-t) \frac{m}{M_s} \right]. \end{aligned} \quad (\text{A39})$$

The ratio m/M_s is very small for the ions in the plasma. In the ionic case, the final logarithm above gives only a term of order m/M_s . Thus only the electrons in the plasma give a significant contribution to this high-energy correction. Since the electron density is half the total number density in the completely ionized plasma, we may write

$$4\pi e^2 \beta \langle n_e \rangle_\beta = \frac{1}{2} \kappa_D^2. \quad (\text{A40})$$

The t integration in Eq. (A39) is elementary, and we secure at last

$$\Delta D(\beta, \mu_e) = \langle n_e \rangle \frac{Z \kappa_D^2 \lambda_e^3}{8\pi^3 a_0} I, \quad (\text{A41})$$

in which I is the analytically intractable integral

$$I = - \int_0^\infty \frac{dx}{x^4} \left\{ \sqrt{1+x^2} \ln \left[\sqrt{1+x^2} + x \right] - x \right\} \ln \left| \frac{1-x}{1+x} \right|, \quad (\text{A42})$$

whose numerical integration gives $I = 1.105$.

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